

10781442c.trn

New

1

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NEWS 1 Web Page for STN Seminar Schedule - N. America  
NEWS 2 MAR 15 WPIDS/WPIX enhanced with new FRAGHITSTR display format  
NEWS 3 MAR 16 CASREACT coverage extended  
NEWS 4 MAR 20 MARPAT now updated daily  
NEWS 5 MAR 22 LWPI reloaded  
NEWS 6 MAR 30 RDISCLOSURE reloaded with enhancements  
NEWS 7 APR 02 JICST-EPLUS removed from database clusters and STN  
NEWS 8 APR 30 GENBANK reloaded and enhanced with Genome Project ID field  
NEWS 9 APR 30 CHEMCATS enhanced with 1.2 million new records  
NEWS 10 APR 30 CA/CAplus enhanced with 1870-1889 U.S. patent records  
NEWS 11 APR 30 INPADOC replaced by INPADOCDB on STN  
NEWS 12 MAY 01 New CAS web site launched  
NEWS 13 MAY 08 CA/CAplus Indian patent publication number format defined  
NEWS 14 MAY 14 RDISCLOSURE on STN Easy enhanced with new search and display fields  
NEWS 15 MAY 21 BIOSIS reloaded and enhanced with archival data  
NEWS 16 MAY 21 TOXCENTER enhanced with BIOSIS reload  
NEWS 17 MAY 21 CA/CAplus enhanced with additional kind codes for German patents  
NEWS 18 MAY 22 CA/CAplus enhanced with IPC reclassification in Japanese patents  
NEWS 19 JUN 27 CA/CAplus enhanced with pre-1967 CAS Registry Numbers  
NEWS 20 JUN 29 STN Viewer now available  
NEWS 21 JUN 29 STN Express, Version 8.2, now available  
NEWS 22 JUL 02 LEMBASE coverage updated  
NEWS 23 JUL 02 LMEDLINE coverage updated  
NEWS 24 JUL 02 SCISEARCH enhanced with complete author names  
NEWS 25 JUL 02 CHEMCATS accession numbers revised  
NEWS 26 JUL 02 CA/CAplus enhanced with utility model patents from China  
  
NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,  
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.  
  
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FILE 'HOME' ENTERED AT 14:11:14 ON 12 JUL 2007

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

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**STRUCTURE FILE UPDATES:** 11 JUL 2007 HIGHEST RN 942193-36-4  
**DICTIONARY FILE UPDATES:** 11 JUL 2007 HIGHEST RN 942193-36-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

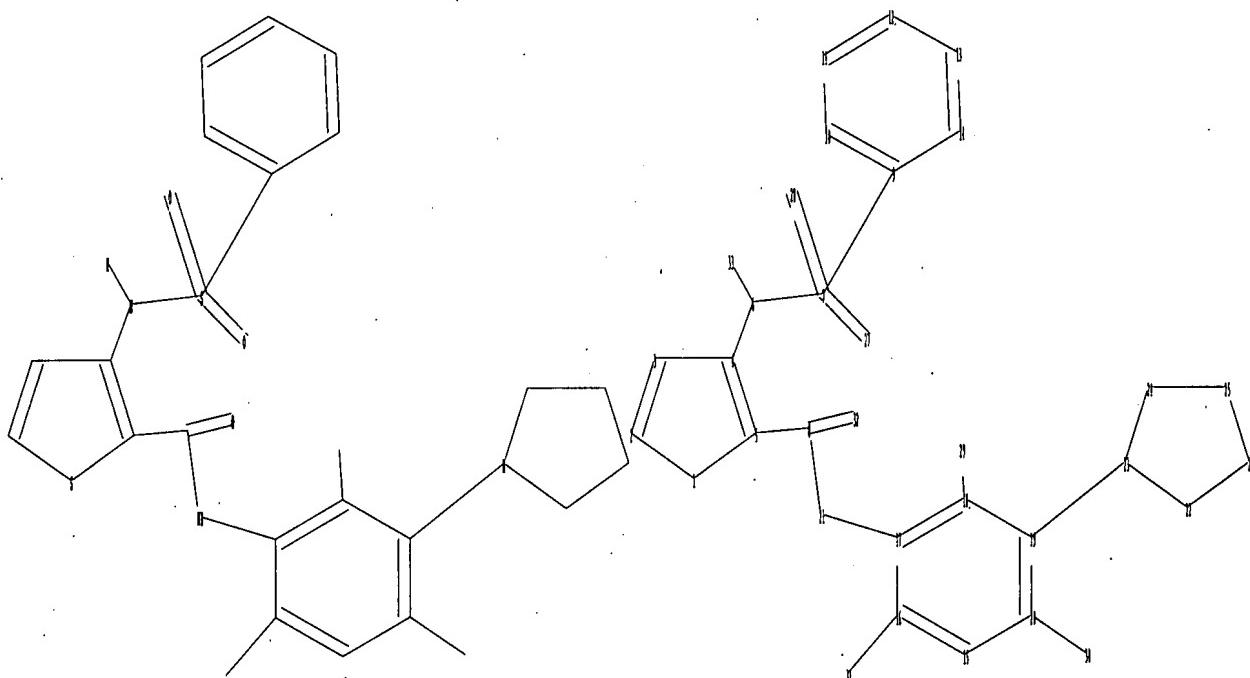
**TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006**

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stnqen/stndoc/properties.html>

=>  
Uploading C:\Program Files\Stnexp\Queries\10781442c.str



chain nodes :

6 7 8 21 27 28 29 30 31 32 33

ring nodes :

1 2 3 4 5 9 10 11 12 13 14 15 16 17 18 19 20 22 23 24 25 26

chain bonds :

4-6 5-8 6-7 6-33 7-9 7-27 7-28 8-21 8-32 16-31 17-21 18-29 19-23 20-30

ring bonds :

1-2 1-5 2-3 3-4 4-5 9-10 9-14 10-11 11-12 12-13 13-14 15-16 15-20

16-17 17-18 18-19 19-20 22-23 22-26 23-24 24-25 25-26

exact/norm bonds :

4-6 6-7 7-9 7-27 7-28 8-21 8-32 17-21 19-23 22-23 23-24

exact bonds :

1-2 1-5 2-3 3-4 4-5 5-8 6-33 16-31 18-29 20-30 22-26 24-25 25-26

normalized bonds :

9-10 9-14 10-11 11-12 12-13 13-14 15-16 15-20 16-17 17-18 18-19 19-20

isolated ring systems :

containing 1 : 9 : 15 : 22 :

Match level :

 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:Atom 10:Atom  
 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom  
 20:Atom 21:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS 28:CLASS  
 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS

L1 STRUCTURE UPLOADED

=&gt; d 11

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L1 HAS NO ANSWERS  
L1 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> S 11  
SAMPLE SEARCH INITIATED 14:12:36 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 25 TO ITERATE

100.0% PROCESSED 25 ITERATIONS 1 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 200 TO 800  
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> S 11 sss full  
FULL SEARCH INITIATED 14:12:42 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 481 TO ITERATE

100.0% PROCESSED 481 ITERATIONS 24 ANSWERS  
SEARCH TIME: 00.00.01

L3 24 SEA SSS FUL L1

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.55	172.76

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FILE COVERS 1907 - 12 Jul 2007 VOL 147 ISS 3  
FILE LAST UPDATED: 11 Jul 2007 (20070711/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> s 13

L4

2 L3

=> d 14 ibib abs hitstr tot

L4 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:185392 HCAPLUS

DOCUMENT NUMBER: 142:280229

TITLE: A preparation of urotensin II receptor antagonists and CCR-9 antagonists

INVENTOR(S): Wu, Chengde; Anderson, C. Eric; Bui, Huong; Gao, Dixin; Kassir, Jamal; Li, Wen; Wang, Junmei; Biediger, Ronald; Chen, Jie; Market, Robert V.

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 33 pp., Cont.-in-part of U.S. Ser. No. 781,442.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

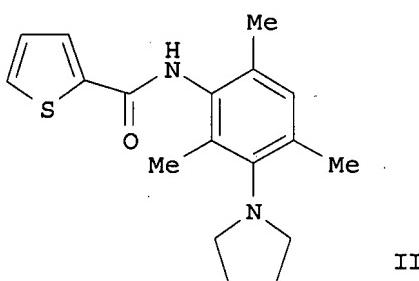
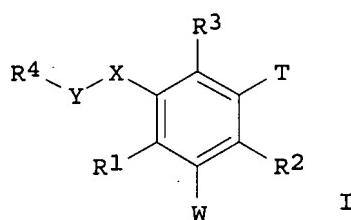
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005049286	A1	20050303	US 2004-924180	20040823
US 2004180892	A1	20040916	US 2004-781442	20040218
PRIORITY APPLN. INFO.:			US 2003-448791P	P 20030220
			US 2004-781442	A2 20040218

OTHER SOURCE(S): MARPAT 142:280229

GI



AB The invention relates to a preparation of urotensin II receptor antagonists and CCR-9 antagonists of formula I [wherein: R1, R2, and R3 are independently

selected from H, halogen, alkyl, aryl, or CN, etc.; X is CH<sub>2</sub>, O, or NH, etc.; Y is SO<sub>2</sub>, C(O), CH<sub>2</sub>SO<sub>2</sub>, NHC(O), or NHSO<sub>2</sub>, etc.; T and W are independently selected from H, (cyclo)alkyl, alkoxy, aryl, or halogen, etc.; R<sub>4</sub> is aryl, heterocyclyl, or cycloalkyl]. For instance, thiophenecarboxamide derivative II was prepared via amidation of thiophene-2-carboxylic acid by [2,4,6-trimethyl-3-(pyrrolidin-1-yl)phenyl]amine. The invention compds. were tested for inhibition of human urotensin II-induced Ca<sup>2+</sup> mobilization in UTR cells (IC<sub>50</sub> > 0.5 μM).

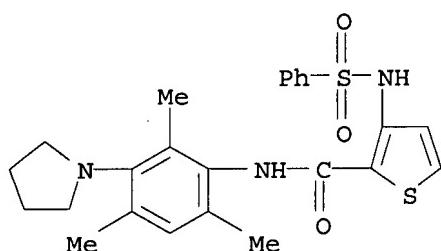
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 847414-39-5P 847414-40-8P 847414-41-9P  
 847414-42-0P 847414-43-1P 847414-44-2P  
 847414-45-3P 847414-46-4P 847414-47-5P  
 847414-48-6P 847414-49-7P 847414-50-0P  
 847414-51-1P 847414-52-2P 847414-53-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of urotensin II receptor antagonists and CCR-9 antagonists)

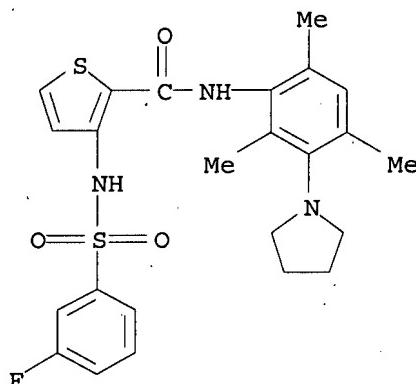
RN 749268-38-0 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[(phenylsulfonyl)amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



RN 847414-30-6 HCAPLUS

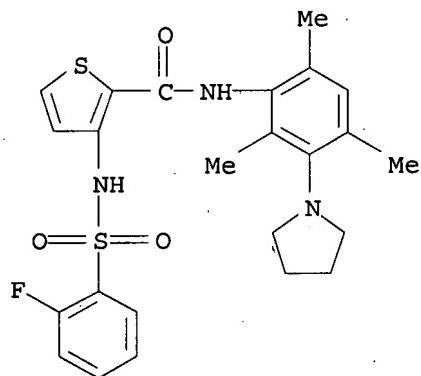
CN 2-Thiophenecarboxamide, 3-[[3-fluorophenyl)sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



RN 847414-31-7 HCAPLUS

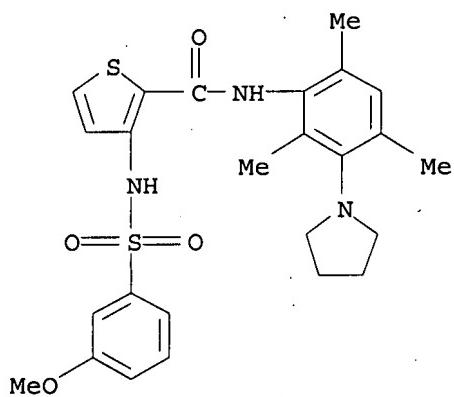
CN 2-Thiophenecarboxamide, 3-[(2-fluorophenyl)sulfonyl]amino]-N-[2,4,6-

trimethyl-3-(1-pyrrolidinyl)phenyl- (9CI) (CA INDEX NAME)



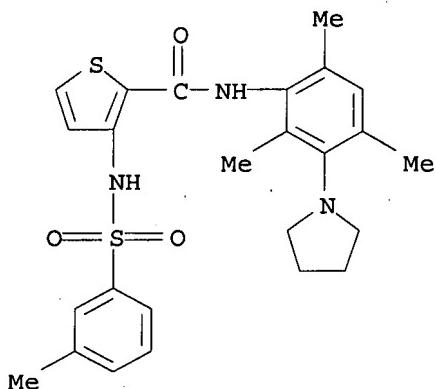
RN 847414-33-9 HCPLUS

CN 2-Thiophenecarboxamide, 3-[[[(3-methoxyphenyl)sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



RN 847414-34-0 HCPLUS

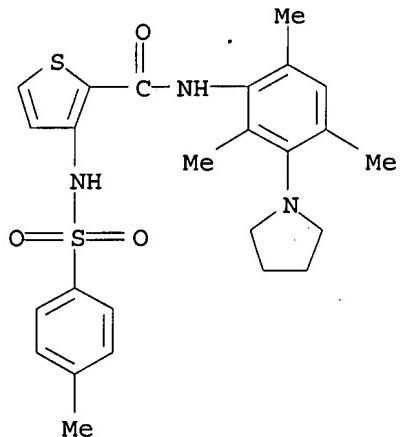
CN 2-Thiophenecarboxamide, 3-[[[(3-methylphenyl)sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



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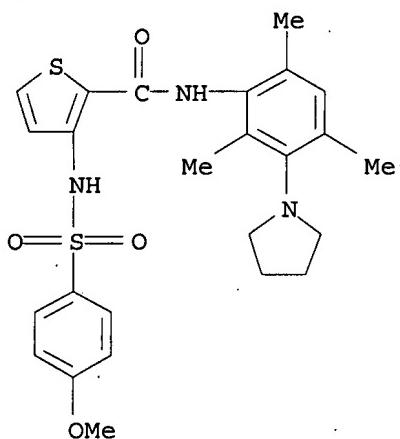
RN 847414-35-1 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[4-methylphenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



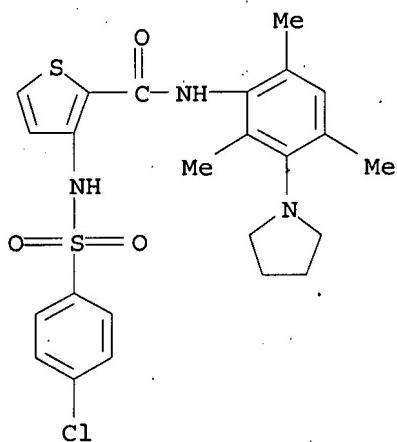
RN 847414-36-2 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[4-methoxyphenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



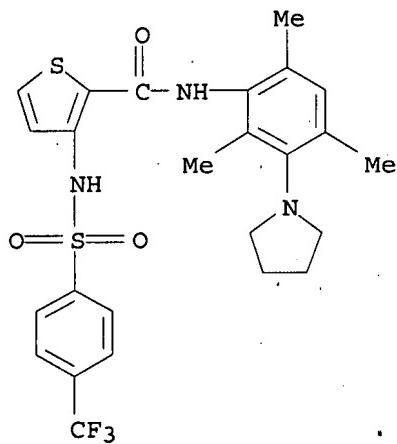
RN 847414-37-3 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[4-chlorophenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



RN 847414-38-4 HCAPLUS

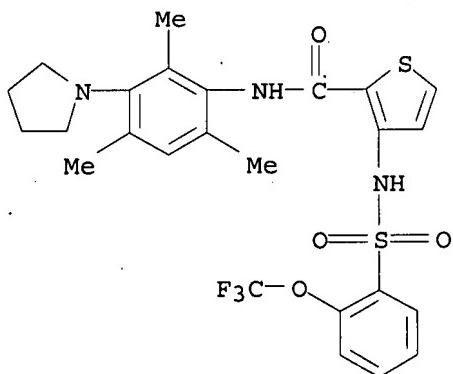
CN 2-Thiophenecarboxamide, 3-[[[4-(trifluoromethyl)phenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



RN 847414-39-5 HCAPLUS

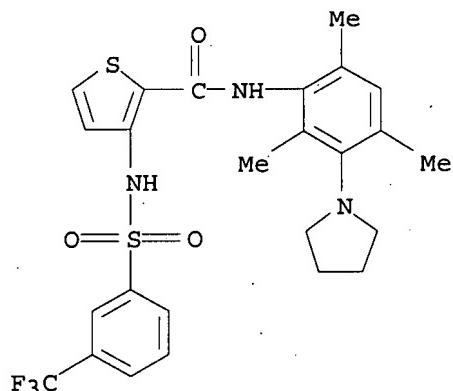
CN 2-Thiophenecarboxamide, 3-[[[2-(trifluoromethoxy)phenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)

10781442c.trn



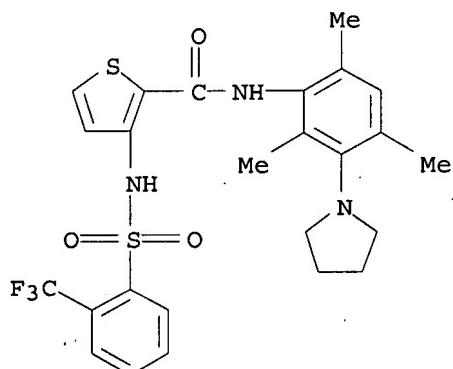
RN 847414-40-8 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[3-(trifluoromethyl)phenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



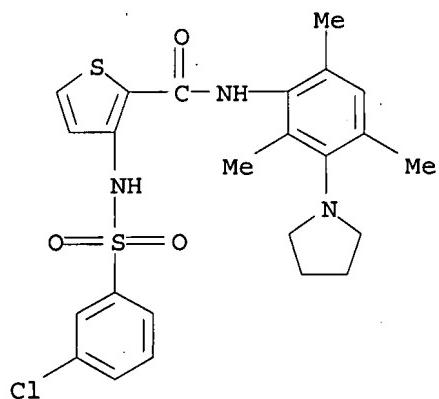
RN 847414-41-9 HCAPLUS

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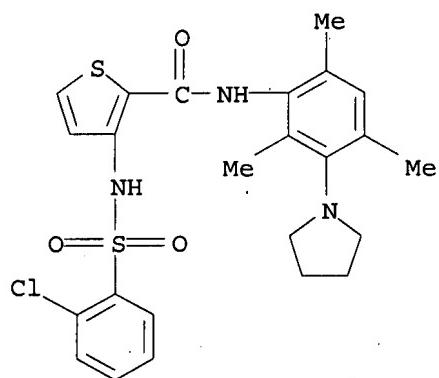
RN 847414-42-0 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[(3-chlorophenyl)sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



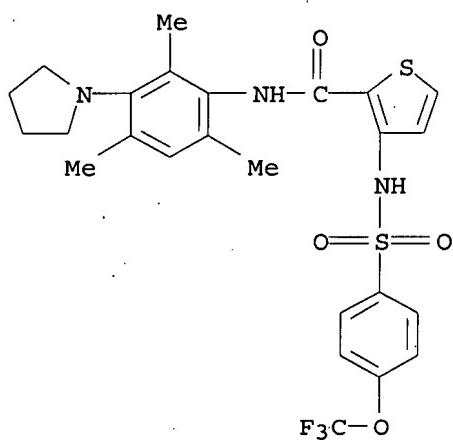
RN 847414-43-1 HCPLUS

CN 2-Thiophenecarboxamide, 3-[[[2-chlorophenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



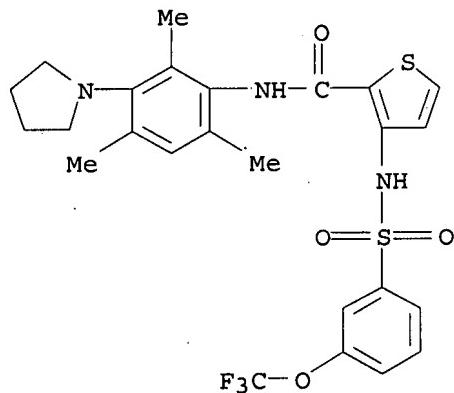
RN 847414-44-2 HCPLUS

CN 2-Thiophenecarboxamide, 3-[[[4-(trifluoromethoxy)phenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



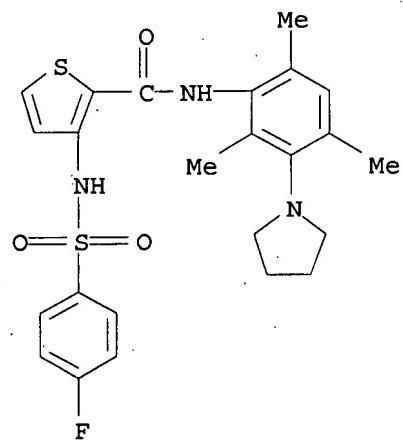
RN 847414-45-3 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[3-(trifluoromethoxy)phenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



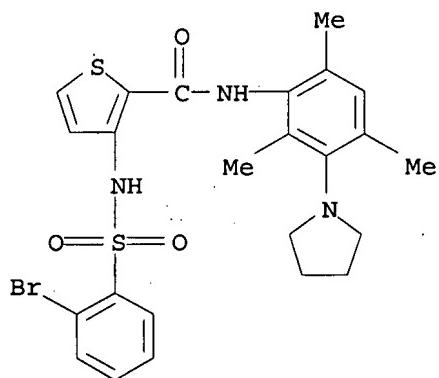
RN 847414-46-4 HCAPLUS

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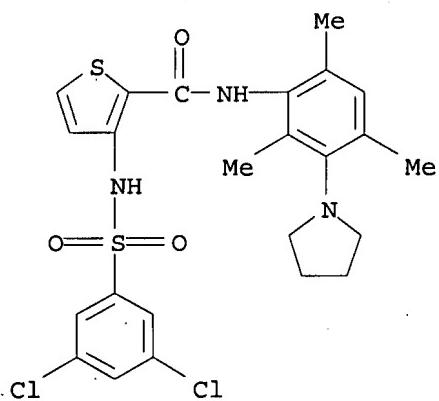
RN 847414-47-5 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[2-bromophenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



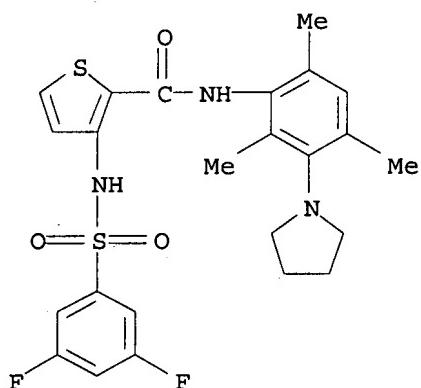
RN 847414-48-6 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[3,5-dichlorophenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



RN 847414-49-7 HCAPLUS

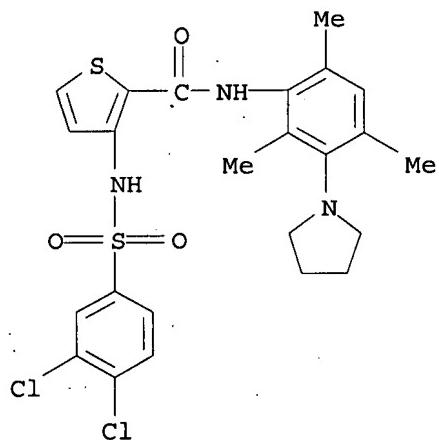
CN 2-Thiophenecarboxamide, 3-[[[3,5-difluorophenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



RN 847414-50-0 HCAPLUS

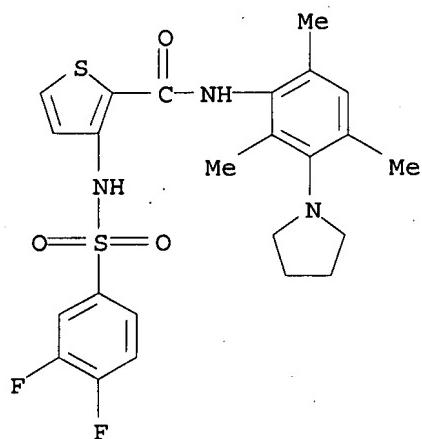
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trimethyl-3-(1-pyrrolidinyl)phenyl- (9CI) (CA INDEX NAME)



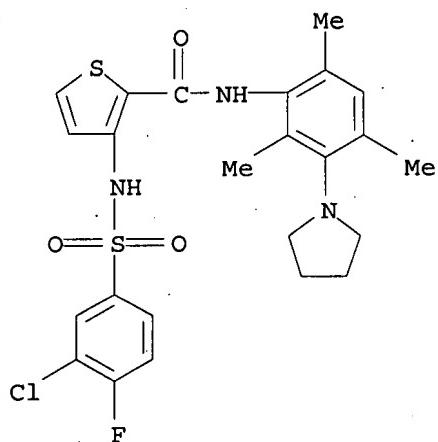
RN 847414-51-1 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[(3,4-difluorophenyl)sulfonyl]amino-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



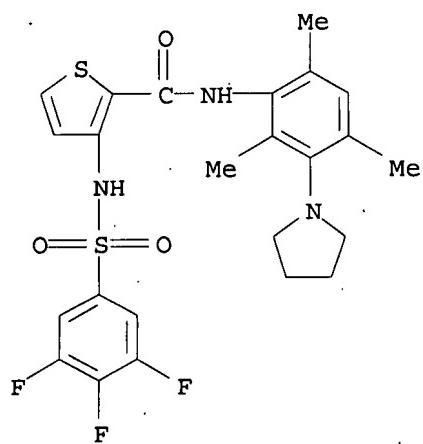
RN 847414-52-2 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[(3-chloro-4-fluorophenyl)sulfonyl]amino-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



RN 847414-53-3 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[(3,4,5-trifluorophenyl)sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:718308 HCAPLUS

DOCUMENT NUMBER: 141:243188

TITLE: Preparation of phenylenediamine and thiophene carboxylic amide derivatives as urotensin-II receptor antagonists and CCR-9 antagonists

INVENTOR(S): Wu, Chengde; Anderson, Eric C.; Bui, Huong; Gao, Dixin; Kassir, Jamal; Li, Wen; Wang, Junmei; Market, Robert V.

PATENT ASSIGNEE(S): Encysive Pharmaceuticals Inc., USA

SOURCE: PCT Int. Appl., 84 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

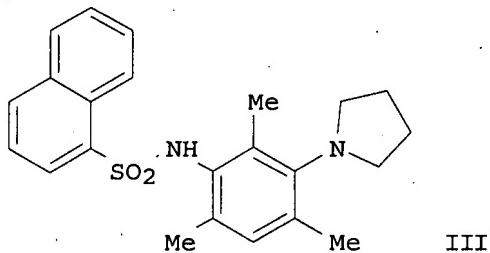
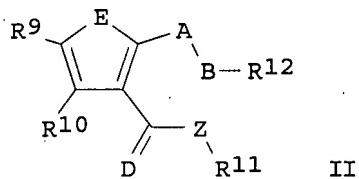
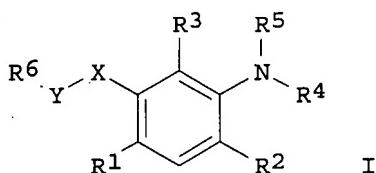
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004073634	A2	20040902	WO 2004-US4645	20040218
WO 2004073634	A3	20060914		
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EP 1610753	A2	20060104	EP 2004-712313	20040218
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JP 2006519785	T	20060831	JP 2006-503636	20040218
PRIORITY APPLN. INFO.: US 2003-448791P P 20030220 WO 2004-US4645 W 20040218				

OTHER SOURCE(S): MARPAT 141:243188  
GI



AB The title compds. I and II [R1, R2, R3 = H, halo, alkyl, aryl, aralkyl, CN, CF<sub>3</sub>, etc.; X = N, CH<sub>2</sub>, or O; Y = SO<sub>2</sub>, CO, CH<sub>2</sub>SO<sub>2</sub>, CH<sub>2</sub>CO, NHCO, OCO, or NHSO<sub>2</sub>; R4 = alkyl, aralkyl or (hetero)aryl, R5 = R1, or Z-NR7R8, or R4, R5 taken together with N can form a 5 or 6 membered ring; Z = (CH<sub>2</sub>)<sub>n</sub>, where n = 0-6; R6 = (hetero)aryl, Z-NR7R8; R7, R8 = H, alkyl, aryl, aralkyl or together with N form a pyrrolidine, piperazine, piperidine, or morpholine ring; E = substituted amino, O, S, CR13=CR14, or CR13=N, where R13, R14 = alkyl, (hetero)aryl, halo, OH, alkoxy, etc.; D = substituted amino, O, or

S; Z = NR15 or CR15R15 where each R15 = H, alkyl, aryl, or heteroaryl; A = (substituted)amino, CO, or SO2; when A = (substituted)amino, B = SO2, CO2, or C16R16, where R16 = H, alkyl, aryl, or heteroaryl; when A = CO or SO2, B = (substituted)amino; R9, R10 = H, alkyl, (hetero)aryl, halo, OH, Alkoxy, or (substituted)amino; R11, R12 = H, alkyl, or (hetero)aryl] were prepared as urotensin-II receptor antagonists and CCR-9 antagonists for the treatment of congestive heart failure, stroke, ischemic heart disease, etc. For example, reaction of 2,4,6-trimethyl-3-pyrrolidin-1-yl-phenylamine (preparation given) with 1-naphthalenesulfonyl chloride yielded compound III. The latter showed an IC50 = 10  $\mu$ M in the assay of human urotensin-II-induced CA2+ mobilization in UTR cells.

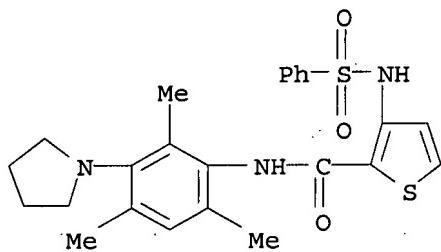
IT 749268-38-0P, 3-Benzenesulfonylamino-N-(2,4,6-trimethyl-3-pyrrolidin-1-yl-phenyl)-thiophene-2-carboxamide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Preparation of phenylenediamine and thiophene carboxylic amide derivs. as urotensin-II receptor antagonists and CCR-9 antagonists)

RN 749268-38-0 HCAPLUS

CN 2-Thiophencarboxamide, 3-[(phenylsulfonyl)amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



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COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	20.94	193.70

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.56	-1.56

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DICTIONARY FILE UPDATES: 11 JUL 2007 HIGHEST RN 942193-36-4

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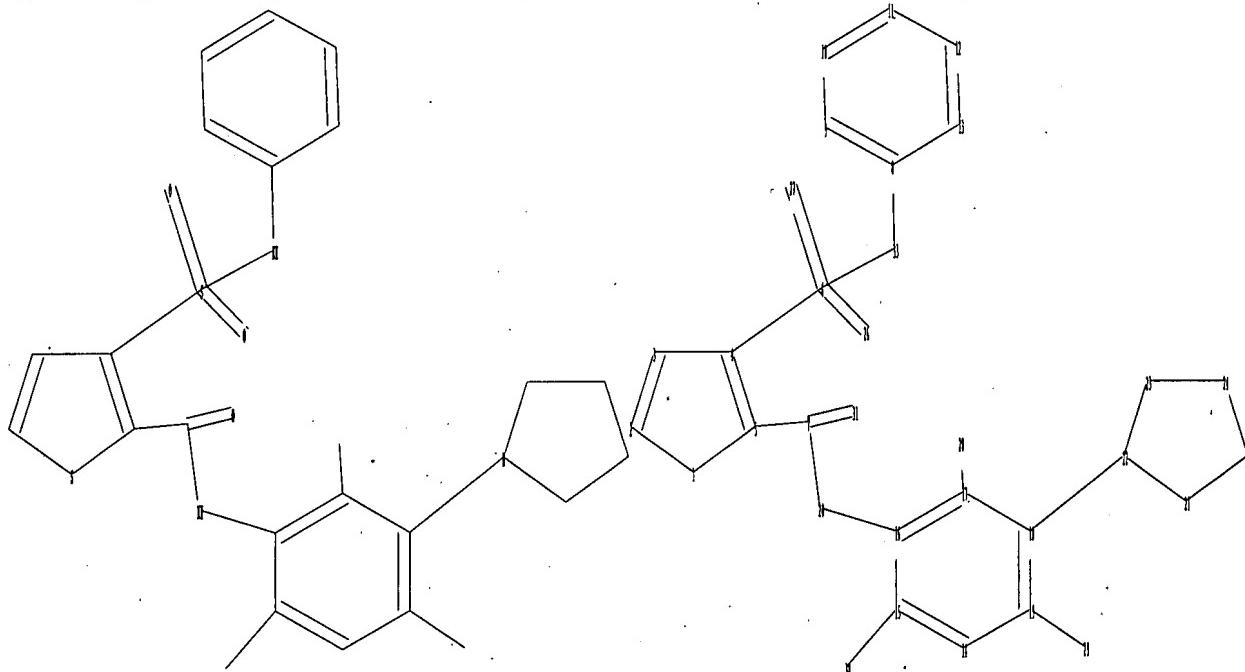
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=>

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chain nodes :

6 7 20 26 27 28 29 30 31 33

ring nodes :

1 2 3 4 5 8 9 10 11 12 13 14 15 16 17 18 19 21 22 23 24 25

chain bonds :

4-6 5-7 6-27 6-26 6-33 7-20 7-31 8-33 15-30 16-20 17-28 18-22 19-29

ring bonds :

1-2 1-5 2-3 3-4 4-5 8-9 8-13 9-10 10-11 11-12 12-13 14-15 14-19 15-16

16-17 17-18 18-19 21-22 21-25 22-23 23-24 24-25

exact/norm bonds :

4-6 6-27 6-26 6-33 7-20 7-31 8-33 16-20 18-22 21-22 22-23

exact bonds :

1-2 1-5 2-3 3-4 4-5 5-7 15-30 17-28 19-29 21-25 23-24 24-25

normalized bonds :

8-9 8-13 9-10 10-11 11-12 12-13 14-15 14-19 15-16 16-17 17-18 18-19

isolated ring systems :

containing 1 : 8 : 14 : 21 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom

20:CLASS 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 27:CLASS 28:CLASS

07/12/2007 Page 18:CLASS

10781442c.trn

L5 STRUCTURE UPLOADED

=> d 15  
L5 HAS NO ANSWERS  
L5 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

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=> s 15  
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SAMPLE SCREEN SEARCH COMPLETED - 40 TO ITERATE

100.0% PROCESSED 40 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 421 TO 1179  
PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=> s 15 sss full  
FULL SEARCH INITIATED 14:16:00 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 800 TO ITERATE

100.0% PROCESSED 800 ITERATIONS 4 ANSWERS  
SEARCH TIME: 00.00.01

L7 4 SEA SSS FUL L5

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COST IN U.S. DOLLARS		
FULL ESTIMATED COST	172.10	365.80
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CA SUBSCRIBER PRICE	0.00	-1.56

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FILE COVERS 1907 - 12 Jul 2007 VOL 147 ISS 3  
FILE LAST UPDATED: 11 Jul 2007 (20070711/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

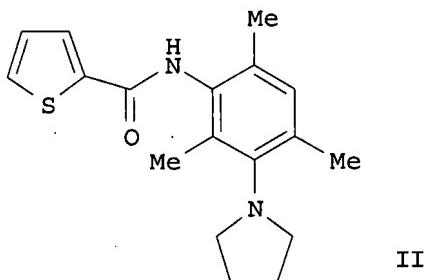
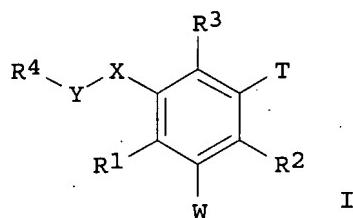
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L8            2 L7

=> d 18 ibib abs hitstr tot

L8 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2005:185392 HCAPLUS  
DOCUMENT NUMBER: 142:280229  
TITLE: A preparation of urotensin II receptor antagonists and CGRP-9 antagonists  
INVENTOR(S): Wu, Chengde; Anderson, C. Eric; Bui, Huong; Gao, Dixin; Kassir, Jamal; Li, Wen; Wang, Junmei; Biediger, Ronald; Chen, Jie; Market, Robert V.  
PATENT ASSIGNEE(S): USA  
SOURCE: U.S. Pat. Appl. Publ., 33 pp., Cont.-in-part of U.S. Ser. No. 781,442.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005049286	A1	20050303	US 2004-924180	20040823
US 2004180892	A1	20040916	US 2004-781442	20040218
PRIORITY APPLN. INFO.:			US 2003-448791P	P 20030220
			US 2004-781442	A2 20040218

OTHER SOURCE(S): MARPAT 142:280229  
GI



**AB** The invention relates to a preparation of urotensin II receptor antagonists and CCR-9 antagonists of formula I [wherein: R1, R2, and R3 are independently selected from H, halogen, alkyl, aryl, or CN, etc.; X is CH<sub>2</sub>, O, or NH, etc.; Y is SO<sub>2</sub>, C(O), CH<sub>2</sub>SO<sub>2</sub>, NHC(O), or NHSO<sub>2</sub>, etc.; T and W are independently selected from H, (cyclo)alkyl, alkoxy, aryl, or halogen, etc.; R<sub>4</sub> is aryl, heterocyclyl, or cycloalkyl]. For instance, thiophenecarboxamide derivative II was prepared via amidation of thiophene-2-carboxylic acid by [2,4,6-trimethyl-3-(pyrrolidin-1-yl)phenyl]amine. The invention compds. were tested for inhibition of human urotensin II-induced Ca<sup>2+</sup> mobilization in UTR cells (IC<sub>50</sub> > 0.5 μM).

**IT** 749268-37-9P 847414-62-4P 847414-63-5P

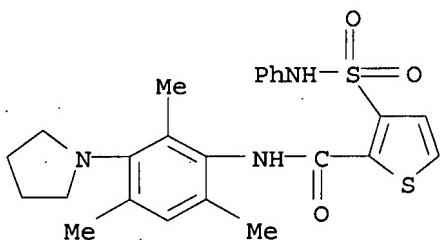
847414-64-6P

**RL:** PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of urotensin II receptor antagonists and CCR-9 antagonists)

**RN** 749268-37-9 HCAPLUS

**CN** 2-Thiophenecarboxamide, 3-[(phenylamino)sulfonyl]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)

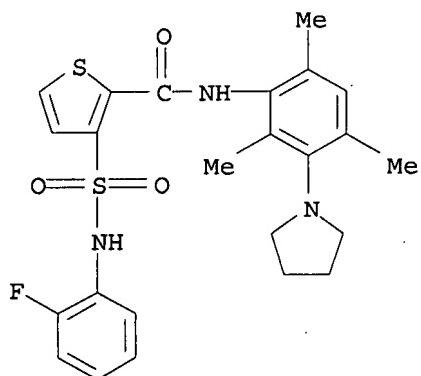


**RN** 847414-62-4 HCAPLUS

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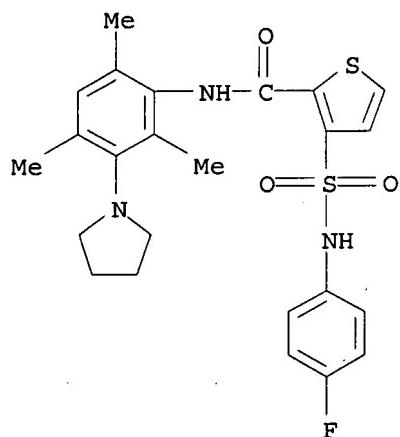
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trimethyl-3-(1-pyrrolidinyl)phenyl- (9CI) (CA INDEX NAME)



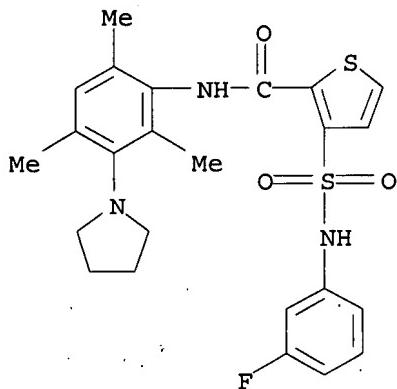
RN 847414-63-5 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[4-fluorophenyl)amino]sulfonyl]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



RN 847414-64-6 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[3-fluorophenyl)amino]sulfonyl]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



L8 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:718308 HCAPLUS

DOCUMENT NUMBER: 141:243188

TITLE: Preparation of phenylenediamine and thiophene carboxylic amide derivatives as urotensin-II receptor antagonists and CCR-9 antagonists

INVENTOR(S): Wu, Chengde; Anderson, Eric C.; Bui, Huong; Gao, Daxin; Kassir, Jamal; Li, Wen; Wang, Junmei; Market, Robert V.

PATENT ASSIGNEE(S): Encysive Pharmaceuticals Inc., USA

SOURCE: PCT Int. Appl., 84 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

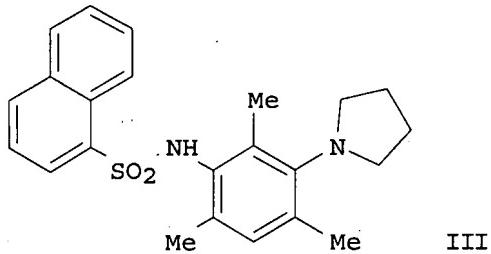
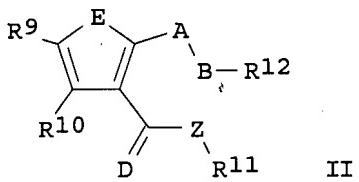
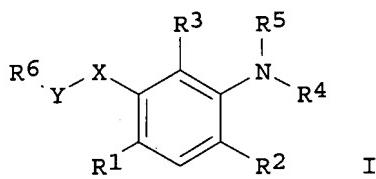
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004073634	A3	20060914		
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EP 1610753	A2	20060104	EP 2004-712313	20040218
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006519785	T	20060831	JP 2006-503636	20040218
PRIORITY APPLN. INFO.:			US 2003-448791P	P 20030220
			WO 2004-US4645	W 20040218

OTHER SOURCE(S): MARPAT 141:243188

GI



**AB** The title compds. I and II [R1, R2, R3 = H, halo, alkyl, aryl, aralkyl, CN, CF<sub>3</sub>, etc.; X = N, CH<sub>2</sub>, or O; Y = SO<sub>2</sub>, CO, CH<sub>2</sub>SO<sub>2</sub>, CH<sub>2</sub>CO, NHCO, OCO, or NHSO<sub>2</sub>; R4 = alkyl, aralkyl or (hetero)aryl, R5 = R1, or Z-NR7R8, or R4, R5 taken together with N can form a 5 or 6 membered ring; Z = (CH<sub>2</sub>)<sub>n</sub>, where n = 0-6; R6 = (hetero)aryl, Z-NR7R8; R7, R8 = H, alkyl, aryl, aralkyl or together with N form a pyrrolidine, piperazine, piperidine, or morpholine ring; E = substituted amino, O, S, CR13=CR14, or CR13=N, where R13, R14 = alkyl, (hetero)aryl, halo, OH, alkoxy, etc.; D = substituted amino, O, or S; Z = NR15 or CR15R15 where each R15 = H, alkyl, aryl, or heteroaryl; A = (substituted)amino, CO, or SO<sub>2</sub>; when A = (substituted)amino, B = SO<sub>2</sub>, CO<sub>2</sub>, or C<sub>16</sub>R<sub>16</sub>, where R<sub>16</sub> = H, alkyl, aryl, or heteroaryl; when A = CO or SO<sub>2</sub>, B = (substituted)amino; R9, R10 = H, alkyl, (hetero)aryl, halo, OH, Alkoxy, or (substituted)amino; R11, R12 = H, alkyl, or (hetero)aryl] were prepared as urotensin-II receptor antagonists and CCR-9 antagonists for the treatment of congestive heart failure, stroke, ischemic heart disease, etc. For example, reaction of 2,4,6-trimethyl-3-pyrrolidin-1-yl-phenylamine (preparation given) with 1-naphthalenesulfonyl chloride yielded compound III. The latter showed an IC<sub>50</sub> = 10 μM in the assay of human urotensin-II-induced CA<sub>2+</sub> mobilization in UTR cells.

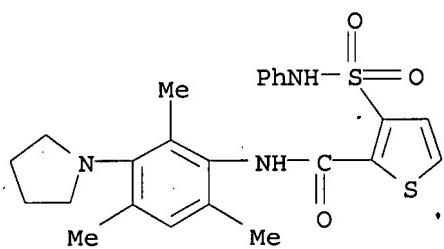
**IT** 749268-37-9P, 3-Phenylaminosulfonyl-N-(2,4,6-trimethyl-3-pyrrolidin-1-yl-phenyl)-thiophene-2-carboxamide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Preparation of phenylenediamine and thiophene carboxylic amide derivs. as urotensin-II receptor antagonists and CCR-9 antagonists)

**RN** 749268-37-9 HCAPLUS

**CN** 2-Thiophencarboxamide, 3-[(phenylamino)sulfonyl]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



=> log y  
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	26.14	391.94

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE ENTRY	TOTAL SESSION
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NEWS 12 MAY 01 New CAS web site launched  
NEWS 13 MAY 08 CA/CAplus Indian patent publication number format defined  
NEWS 14 MAY 14 RDISCLOSURE on STN Easy enhanced with new search and display fields  
NEWS 15 MAY 21 BIOSIS reloaded and enhanced with archival data  
NEWS 16 MAY 21 TOXCENTER enhanced with BIOSIS reload  
NEWS 17 MAY 21 CA/CAplus enhanced with additional kind codes for German patents  
NEWS 18 MAY 22 CA/CAplus enhanced with IPC reclassification in Japanese patents  
NEWS 19 JUN 27 CA/CAplus enhanced with pre-1967 CAS Registry Numbers  
NEWS 20 JUN 29 STN Viewer now available  
NEWS 21 JUN 29 STN Express, Version 8.2, now available  
NEWS 22 JUL 02 LEMBASE coverage updated  
NEWS 23 JUL 02 LMEDLINE coverage updated  
NEWS 24 JUL 02 SCISEARCH enhanced with complete author names  
NEWS 25 JUL 02 CHEMCATS accession numbers revised  
NEWS 26 JUL 02 CA/CAplus enhanced with utility model patents from China  
  
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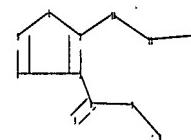
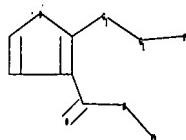
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<http://www.cas.org/support/stnqen/stndoc/properties.html>

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chain nodes :

6 7 8 9 10 11 12

ring nodes :

1 2 3 4 5

chain bonds :

2-10 3-6 6-7 6-9 7-8 10-11 11-12

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

2-10 6-7 6-9 10-11 11-12

exact bonds :

1-2 1-5 2-3 3-4 3-6 4-5 7-8

isolated ring systems :

containing 1 :

G1:SO2,NH,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS  
10:CLASS 11:CLASS 12:CLASS

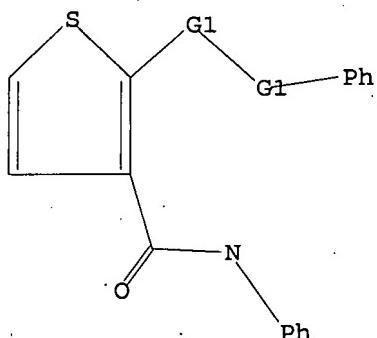
L1 STRUCTURE UPLOADED

=> D L1

L1 HAS NO ANSWERS

10781442.trn

L1 STR



G1 SO2, NH, N

Structure attributes must be viewed using STN Express query preparation.

=> S L1

SAMPLE SEARCH INITIATED 13:19:19 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 159 TO ITERATE

100.0% PROCESSED 159 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 2424 TO 3936

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

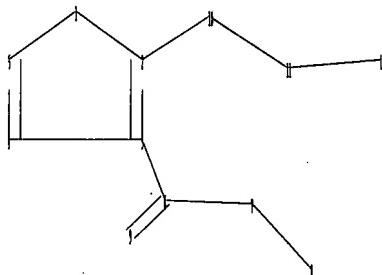
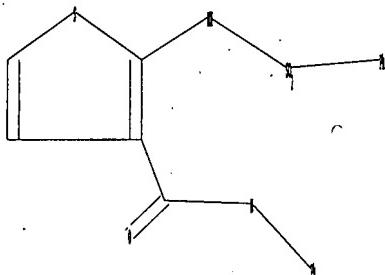
=> S L1 SSS FULL  
FULL SEARCH INITIATED 13:19:26 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 3278 TO ITERATE

100.0% PROCESSED 3278 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

L3 0 SEA SSS FUL L1

=>  
Uploading C:\Program Files\Stnexp\Queries\10781442a.str



chain nodes :

6 7 8 9 10 11 12

10781442.trn

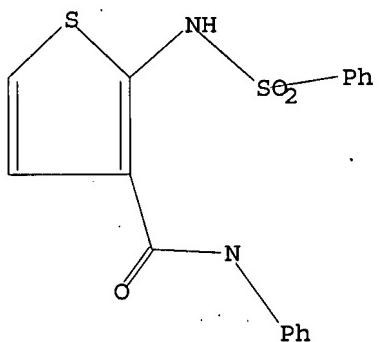
ring nodes :  
1 2 3 4 5  
chain bonds :  
2-10 3-6 6-7 6-9 7-8 10-11 11-12  
ring bonds :  
1-2 1-5 2-3 3-4 4-5  
exact/norm bonds :  
2-10 6-7 6-9 10-11  
exact bonds :  
1-2 1-5 2-3 3-4 3-6 4-5 7-8 11-12  
isolated ring systems :  
containing 1 :

G1:SO2,NH,N

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS  
10:CLASS 11:CLASS 12:CLASS

L4 STRUCTURE UPLOADED

=> d 14  
L4 HAS NO ANSWERS  
L4 STR



G1 SO2,NH,N

Structure attributes must be viewed using STN Express query preparation.

=> s 14  
SAMPLE SEARCH INITIATED 13:22:32 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 14 TO ITERATE

100.0% PROCESSED 14 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 56 TO 504  
PROJECTED ANSWERS: 0 TO 0

10781442.trn

L5 0 SEA SSS SAM L4

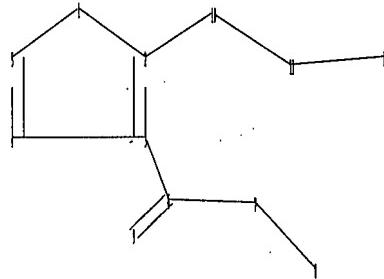
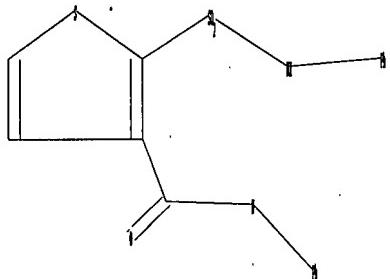
=> s 14 sss full  
FULL SEARCH INITIATED 13:22:38 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 351 TO ITERATE

100.0% PROCESSED 351 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

L6 0 SEA SSS FUL L4

=>  
Uploading C:\Program Files\Stnexp\Queries\10781442b.str



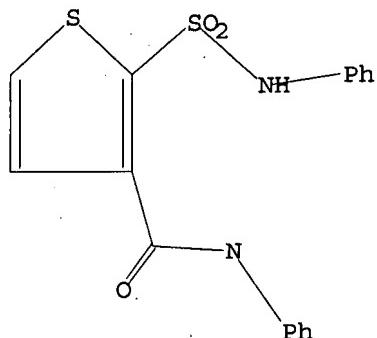
chain nodes :  
6 7 8 9 10 11 12  
ring nodes :  
1 2 3 4 5  
chain bonds :  
2-10 3-6 6-7 6-9 7-8 10-11 11-12  
ring bonds :  
1-2 1-5 2-3 3-4 4-5  
exact/norm bonds :  
6-7 6-9 10-11  
exact bonds :  
1-2 1-5 2-3 2-10 3-4 3-6 4-5 7-8 11-12  
isolated ring systems :  
containing 1 :

G1:SO2,NH,N

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS  
10:CLASS 11:CLASS 12:CLASS

L7 STRUCTURE UPLOADED

=> d 17  
L7 HAS NO ANSWERS  
L7 STR



G1 SO2,NH,N

Structure attributes must be viewed using STN Express query preparation.

=&gt; s 17

SAMPLE SEARCH INITIATED 13:24:05 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 0 TO 0

PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

=> s 17 sss full  
 FULL SEARCH INITIATED 13:24:11 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 15 TO ITERATE

100.0% PROCESSED 15 ITERATIONS 0 ANSWERS  
 SEARCH TIME: 00.00.01

L9 0 SEA SSS FUL L7

=> log y		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
FULL ESTIMATED COST	ENTRY	SESSION
	519.90	520.11

STN INTERNATIONAL LOGOFF AT 13:25:32 ON 12 JUL 2007